

# Theta and Riemann xi function representations from harmonic oscillator eigensolutions

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## Abstract

From eigensolutions of the harmonic oscillator or Kepler-Coulomb Hamiltonian we extend the functional equation for the Riemann zeta function and develop integral representations for the Riemann xi function that is the completed classical zeta function. A key result provides a basis for generalizing the important Riemann-Siegel integral formula.

## Key words and phrases

harmonic oscillator, Mellin transformation, Hermite polynomial, hypergeometric series, functional equation, theta function, Riemann xi function

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## Introduction

The quantum harmonic oscillator and Kepler-Coulomb problems are of enduring interest to mathematical physics and are in a sense the same problem, for there are many ways to transform one to the other. For example, the 4-dimensional (8-dimensional) harmonic oscillator may be transformed to a 3-dimensional (5-dimensional) Coulomb problem [19, 21]. Many more mappings are realizable, especially for the corresponding radial problems [19]. Therefore, the eigensolutions are very closely related for these two problems with central potentials.

We recall that the eigensolution of the fundamental quantum mechanical problems of the harmonic oscillator and hydrogenic atoms contain Hermite or associated Laguerre polynomials, depending upon the coordinate system used and the spatial dimension (e.g., [24, 10]). Two quantum numbers appear for indexing the energy levels and the angular momentum. These wavefunctions have a wide variety of applicability, including to image processing and the combinatorics of zero-dimensional quantum field theory [10]. Very recently additional analytic properties of these "quantum shapelets" have been expounded [10]. The one-dimensional Coulomb problem has recently reappeared as a model in quantum computing with electrons on liquid helium films [26, 25]. In addition, given the self-reciprocal Fourier transform property of Hermite polynomials, there are several applications in Fourier optics [8, 16]. Hermite and Laguerre polynomials are also important in random matrix theory, especially for determinantal processes [14, 23]. There, the joint probability density function of the eigenvalues of a matrix from one of the Gaussian invariant ensembles

is proportional to a Vandermonde determinant and the orthogonal polynomials form the kernel giving the  $n$ -point correlation function.

The harmonic oscillator Hamiltonian may be given a group theoretic interpretation via the Weil representation of  $SL_2(\mathbb{R})$  [6, 20] and such theory together with that of quantum mechanical commutation relations figures prominently in constructing theta functions [29, 7]. From the Mellin transform of suitable theta functions, one may represent completed zeta functions and one of our main results demonstrates this. Additionally, we present representations of the Riemann xi function that offer the possibility to generalize the very important Riemann-Siegel formula in the theory of the Riemann zeta function [12, 28].

The work of Bump et al. [5, 6, 20] on the Mellin transforms of Hermite and associated Laguerre functions has created significant interest since the zeros of these functions lie only on the critical line  $\text{Re } s = 1/2$ . A complementary point of view is possible within the theory of special functions and in particular, when the Mellin transforms are written in terms of the Gauss hypergeometric function, well known transformation formulae yield functional equations, reciprocity laws, and other properties [11]. As an example, we have very recently shown that the Mellin transform of the Laguerre function  $\mathcal{L}_n^\alpha(x) = x^{\alpha/2} e^{-x/2} L_n^\alpha(x)$ , where  $\alpha > -1$  and  $L_n^\alpha$  is the associated Laguerre polynomial [2, 15, 22], is given by  $M_n^\alpha(s) = 2^{s+\alpha/2} \Gamma(s + \alpha/2) P_n^\alpha(s)$  where  $\Gamma$  is the Gamma function and  $P_n^\alpha(s) = \frac{(1+\alpha)_n}{n!} {}_2F_1(-n, s+\alpha/2; \alpha+1; 2)$ , with  ${}_pF_q$  the generalized hypergeometric function and  $(a)_n = \Gamma(a+n)/\Gamma(a)$  the Pochhammer symbol. In fact, the polynomials  $P_n^\alpha$  are closely related to the symmetric Meixner-

Pollaczek polynomials  $P_n^{(\lambda)}(x, \pi/2)$  [3, 18], and the latter are very useful in random matrix theory [14].

Keating [17] showed how to generalize Riemann's second proof of the functional equation of  $\zeta(s)$  by using Mellin and Fourier transforms of Hermite polynomials. In the next section we illustrate the hypergeometric function point of view of those results. The succeeding section contains our key result. We extend earlier work [5] such that the representations given for the xi function could provide a method to generalize the Riemann-Siegel integral formula of complex analysis. Again we emphasize that these representations are built from the eigensolutions of self-adjoint operators, these operators being the distinguished harmonic oscillator or Coulomb Hamiltonians.

### A family of zeta functions

In Ref. [17] Keating generalized the Jacobi inversion formula, applying Poisson summation to Hermite functions  $\mathcal{H}_n(x) = x^\ell H_n(ax)e^{-cx^2}$ , where  $H_n$  is the Hermite polynomial,  $a \neq 0$ ,  $c = a^2/2$ , and  $\ell = 0, 1, 2, \dots$ . Let the  $\theta$  function  $\omega_{n,\ell}(t)$  be given by

$$\omega_{n,\ell}(t) = \sum_{m=1}^{\infty} m^\ell H_n(\sqrt{2\pi t}m)e^{-\pi m^2 t}. \quad (1)$$

Then we have

**Theorem.** [17] For  $n = 2q$ ,  $n + \ell = 2p$ ,  $p, q, \ell = 0, 1, 2, \dots$ ,  $\text{Re } s > 1 + \ell$ ,

$$\int_0^\infty \omega_{n,\ell}(t)t^{s/2-1}dt = \pi^{-s/2}\Gamma(s/2)\zeta_{n,\ell}(s), \quad (2)$$

where

$$\zeta_{2q,\ell}(s) = (2q)!\zeta(s-\ell) \left[ H_q(s) + \frac{(-1)^q}{q!} \right], \quad (3)$$

and

$$H_q(s) \equiv \sum_{k=0}^{q-1} \frac{(-1)^k 2^{3(q-k)}}{k!(2q-2k)!} \left( \frac{s}{2} \right) \left( \frac{s}{2} + 1 \right) \cdots \left( \frac{s}{2} + q - k - 1 \right). \quad (4)$$

This theorem states that a Mellin transform of  $\omega_{n,\ell}$  gives rise to a family of zeta functions. In this section we first derive the terminating hypergeometric series for the polynomial factor of Eq. (2). We have

**Proposition 1.** For  $q$  a nonnegative integer

$$P_q(s) \equiv H_q(s) + \frac{(-1)^q}{q!} = \frac{(-1)^q}{q!} {}_2F_1 \left( -q, \frac{s}{2}; \frac{1}{2}; 2 \right). \quad (5)$$

Once this form of  $P_q(s)$  is obtained, one may determine the functional equation  $P_q(s) = (-1)^q P_q(1-s)$  and that its zeros are all simple and lie only on  $\text{Re } s = 1/2$  [5, 11].

Proof of Proposition 1. We begin by writing

$$H_q(s) \equiv \sum_{k=0}^{q-1} \frac{(-1)^k 2^{3(q-k)}}{k!(2q-2k)!} \left( \frac{s}{2} \right)_{q-k}, \quad (6)$$

and using  $1/(x-n)! = (-1)^n (-x)_n / \Gamma(x+1)$ ,  $(x)_{n-k} = (-1)^k (x)_n / (1-x-n)_k$ , and the duplication formula  $(x)_{2n} = 2^{2n} (x/2)_n ((x+1)/2)_n$ . These steps give

$$H_q(s) = \frac{(s/2)_q 2^{3q}}{(2q)!} \sum_{k=0}^{q-1} \frac{(-q)_k (1/2 - q)_k}{(1 - s/2 - q)_k} \frac{1}{k!} \frac{1}{2^k}, \quad (7)$$

from which we may read off

$$H_q(s) = \frac{(s/2)_q 2^{3q}}{(2q)!} \left[ {}_2F_1(-q, 1/2 - q; 1 - s/2 - q; 1/2) - \frac{(-q)_q (1/2 - q)_q}{(1 - s/2 - q)_q} \frac{1}{q!} \frac{1}{2^q} \right]. \quad (8)$$

By using  $(-q)_q = (-1)^q q!$  we then have by re-arranging the last term of this equation

$$H_q(s) = \frac{(s/2)_q 2^{3q}}{(2q)!} \left[ {}_2F_1(-q, 1/2 - q; 1 - s/2 - q; 1/2) - \left(-\frac{1}{2}\right)^q \frac{\sin(\pi s/2)}{\sqrt{\pi}} \frac{\Gamma(s/2)}{\Gamma(1/2 - q)} \Gamma(1 - s/2 - q) \right]. \quad (9)$$

The  ${}_2F_1$  function of Eq. (9) can be transformed to another hypergeometric function at argument  $-1/2$ ,  $-1$ , or  $2$ . In particular, if we apply ([15], 9.132.2) we have

$${}_2F_1(-q, 1/2 - q; 1 - s/2 - q; 1/2) = \frac{\Gamma(q + 1/2)}{\pi^{3/2} 2^q} \Gamma(1 - s/2 - q) \sin(\pi s/2) \Gamma(s/2) {}_2F_1(-q, s/2; 1/2; 2) \quad (10a)$$

$$= \frac{(-1)^q \Gamma(q + 1/2)}{\sqrt{\pi} 2^q \Gamma(s/2 + q)} \Gamma(s/2) {}_2F_1(-q, s/2; 1/2; 2). \quad (10b)$$

In obtaining Eq. (10a) we used  $\Gamma(1/2 - q)\Gamma(1/2 + q) = \pi / \cos(\pi q) = (-1)^q \pi$  for  $q$  a nonnegative integer. By then inserting Eq. (10b) into Eq. (9) and re-arranging we have

$$H_q(s) = \frac{2^{2q}}{(2q)!} \frac{\Gamma(q + 1/2)}{\sqrt{\pi}} (-1)^q [{}_2F_1(-q, s/2; 1/2; 2) - 1]. \quad (11)$$

We then use  $\Gamma(q + 1/2) = \sqrt{\pi} (2q - 1)!! / 2^q$  and  $(2q - 1)!! = (2q)! / 2^q q!$  to arrive at

$$H_q(s) = \frac{(-1)^q}{q!} [{}_2F_1(-q, s/2; 1/2; 2) - 1], \quad (12)$$

giving Eq. (5).

**Corollary 1.** By applying the transformation formula [15]  ${}_2F_1(\alpha, \beta; \gamma; z) = (1 - z)^{-\alpha} {}_2F_1\left(\alpha, \gamma - \beta; \gamma; \frac{z}{z-1}\right)$  we immediately find the functional equation  $P_q(s) = (-1)^q P_q(1 - s)$ .

**Corollary 2.** From the functional equation we have  $P_q^{(j)}(s) = (-1)^{q+j} P_q^{(j)}(1 - s)$  so that  $P_q^{(j)}(1/2) = 0$  when  $q + j$  is an odd integer and in particular  $P_q(1/2) = 0$  when

$q$  is odd. The latter fact may also be found from the  $\alpha = -1/2$  case of the answer to the following question. For what values of  $n$  is  ${}_2F_1(-n, (\alpha + 1)/2; \alpha + 1; 2) = 0$ ? The hypergeometric function here may be written as an  $n$ th divided difference summation and as a result  ${}_2F_1(-n, (\alpha + 1)/2; \alpha + 1; 2) = \Gamma(1/2)\Gamma[-(n + \alpha)/2]/\Gamma(-\alpha/2)\Gamma[(1 - n)/2]$ . The simple poles of the last  $\Gamma$  factor dictate that the  ${}_2F_1$  function vanishes when  $n$  is an odd integer, as expected.

The following subsumes Theorem 3.4 of Keating [17] for special values of the function  $\zeta_{2q,0}(s)$ .

**Proposition 2.** Put  $c_q \equiv (-1)^q(2q)!/q! = H_{2q}(0)$  and let  $B_j$  denote the Bernoulli numbers. For  $n, q = 0, 1, 2, \dots$  and  $m = 1, 2, \dots$  we have

$$(i) \quad \zeta_{2q,0}(s) = c_q {}_2F_1(-q, -s/2; 1/2; 2)\zeta(s),$$

$$(ii) \quad \zeta_{2q,0}(2m) = c_q {}_2F_1(-q, -m; 1/2; 2)(2\pi)^{2m} \frac{(-1)^{m+1} B_{2m}}{2(2m)!},$$

$$(iii) \quad \zeta_{2q,0}(-n) = c_q {}_2F_1(-q, n/2; 1/2; 2) \frac{(-1)^n B_{n+1}}{n+1},$$

and

$$(iv) \quad \zeta'_{2q,0}(s) = c_q \left[ {}_2F_1(-q, s/2; 1/2; 2)\zeta'(s) + \zeta(s) \frac{d}{ds} {}_2F_1(-q, s/2; 1/2; 2) \right],$$

where

$$\begin{aligned} \frac{d}{ds} {}_2F_1(-q, s/2; 1/2; 2) &= \frac{1}{2} \sum_{j=1}^q \frac{(-q)_j}{(1/2)_j} (s/2)_j [\psi(s/2 + j) - \psi(s/2)] \frac{2^j}{j!} \\ &= \frac{1}{2} \sum_{j=1}^q \frac{(-q)_j}{(1/2)_j} (s/2)_j \sum_{k=0}^{j-1} \frac{1}{(s/2 + k)} \frac{2^j}{j!}, \end{aligned} \quad (13)$$

and  $\psi = \Gamma'/\Gamma$  is the digamma function [2, 1, 15]. In particular, we have the values  $\zeta(0) = -1/2$ ,  $\zeta'(0) = -\frac{1}{2} \ln 2\pi$  and (v)

$$\left. \frac{d}{ds} {}_2F_1(-q, s/2; 1/2; 2) \right|_{s=0} = \frac{1}{2} \sum_{j=1}^q \frac{(-q)_j}{(1/2)_j} \frac{2^j}{j} = -2q {}_3F_2(1-q, 1, 1; 3/2, 2; 2). \quad (14)$$

Proof of Proposition 2. Parts (i), (ii), and (iii) are obvious from Eqs. (3) and (5) and the value of the Riemann zeta function at the negative integers or at the positive even integers. Part (iii) follows by writing the series form of the function  ${}_2F_1$  and using the derivative of the Pochhammer symbol  $(d/dz)(a)_n = (a)_n[\psi(a+n) - \psi(a)]$ . The second line of Eq. (13) follows by applying the functional equation of the digamma function [15].

Part (v) can be obtained as the limit  $s \rightarrow 0$  of the result of (iv). We provide another proof using a representation of the Pochhammer symbol in terms of Stirling numbers of the first kind  $s(j, k)$  [1]. We have

$$(z)_n = \prod_{k=1}^n (z + k - 1) = \sum_{k=0}^n (-1)^{n-k} s(n, k) z^k. \quad (15)$$

Therefore we have  $(d/dz)(z)_n|_{z=0} = (n-1)!$ , where we used  $s(n, 1) = (-1)^{n-1}(n-1)!$ . Using this fact in the series form of  ${}_2F_1$  gives the first equality in Eq. (14). For the second equality in Eq. (14) we first shift the summation index in the previous one:

$$\left. \frac{d}{ds} {}_2F_1(-q, s/2; 1/2; 2) \right|_{s=0} = \sum_{j=0}^{q-1} \frac{(-q)_{j+1}}{(1/2)_{j+1}} \frac{2^j}{(j+1)}. \quad (16)$$

We then use  $1/(j+1) = (1)_j/(2)_j$ , apply the property  $(a)_{j+1} = a(a+1)_j$ , and the rest of Eq. (14) follows.



**Remarks.** Part (iii) of the Proposition covers the trivial zeros of the zeta function when  $n = 2m$  is an even integer. In regard to part (iv),  $\zeta'(s)$  is often easily found in terms of  $\zeta(s)$  itself from the functional equation. For instance, we have  $\zeta'(-2n) = (-1)^n(2n)!\zeta(2n+1)/2(2\pi)^{2n}$  for  $n = 1, 2, \dots$ . By the method of part (iv) higher derivatives of  $\zeta_{2q,0}(s)$  may be computed.

### Representation of the Riemann xi function

Similarly to the  $\ell = 0$  case of Eq. (1), we put  $\theta_j(x) \equiv \sum_{n=-\infty}^{\infty} f_{2j}(n\sqrt{x})$  where  $f_n(x) = (8\pi)^{-n/2} H_n(\sqrt{2\pi}x) e^{-\pi x^2}$ . We then put

$$\psi_j(x) = \frac{1}{2}[\theta_j(x) - f_{2j}(0)] = \sum_{n=1}^{\infty} f_{2j}(n\sqrt{x}), \quad (17)$$

where explicitly [15]  $f_{2j}(0) = (-1)^j(4\pi)^{-j}(2j-1)!!$ . The functional equation of  $\theta_j$  carries over to  $\psi_j$  so that the following fact is essentially given in Ref. [5].

**Lemma 1.** The function  $\psi_j$  satisfies

$$\psi_j(x) = \frac{(-1)^j}{\sqrt{x}} \psi_j\left(\frac{1}{x}\right) + \frac{1}{2} \left[ \frac{(-1)^j}{\sqrt{x}} - 1 \right] f_{2j}(0). \quad (18)$$

We let as usual  $\xi$  be the Riemann xi function, defined for all complex  $s$  as  $\xi(s) = s(s-1)\pi^{-s/2}\Gamma(s/2)\zeta(s)/2$  and satisfying  $\xi(s) = \xi(1-s)$ . Very closely related to Eq. (5), we put  $p_n(s) = (8\pi)^{-n}(-1)^n(2n)! {}_2F_1(-n, s/2; 1/2; 2)/n!$ . We then have Propositions 3 and 4.

**Proposition 3.** For  $b > 0$  there holds

$$p_j(s) \frac{2\xi(s)}{s(s-1)} = (-1)^j \int_{1/b}^{\infty} x^{-(s+1)/2} \psi_j(x) dx + \int_b^{\infty} \psi_j(x) x^{s/2-1} dx$$

$$-f_{2j}(0) \left[ \frac{b^{s/2}}{s} + \frac{(-1)^j}{1-s} b^{(s-1)/2} \right]. \quad (19)$$

**Proposition 4.** For complex  $b$  with  $|\arg b| < \pi/2$  we have (i)

$$p_j(s) \frac{2\xi(s)}{s(s-1)} = F_b(s) + (-1)^j F_{b^{-1}}(1-s) \quad (20)$$

and (ii) when additionally  $|b| = 1$  we have

$$p_j(s) \frac{2\xi(s)}{s(s-1)} = F_b(s) + (-1)^j \overline{F_b(1-\bar{s})}, \quad (21)$$

where we define

$$F_b(s) = \int_b^\infty \psi_j(x) x^{s/2-1} dx - f_{2j}(0) \frac{b^{s/2}}{s}. \quad (22)$$

When  $j = 0$ ,  $f_0(0) = 1$  and Proposition 3 reduces to the original equation of Riemann [27], while for the special case  $b = 1$  a result of Bump and Ng [5] and Keating [17] (Theorem 3.2) is recovered.

For the proof of Proposition 3 we alternatively evaluate the integral

$$\int_0^\infty \psi_j(x) x^{s/2-1} dx = p_j(s) \pi^{-s/2} \Gamma(s/2) \zeta(s) \quad (23)$$

as  $\int_0^\infty \psi_j(x) x^{s/2-1} dx = \int_0^b \psi_j(x) x^{s/2-1} dx + \int_b^\infty \psi_j(x) x^{s/2-1} dx$ . We then put  $y = 1/x$  in the integral on  $[0, b]$ , apply Lemma 1, and the result Eq. (19) follows.

Proof of Proposition 4. (i) Equation (19) holds not just for positive  $b$  but for all values  $b$  in the wedge  $|\arg b| < \pi/2$  where the theta function  $\psi_j(x)$  is well defined. (ii) The complex conjugate of the function  $F_b(s)$  of Eq. (18) is  $F_{\bar{b}}(\bar{s})$  so that Eq. (21) holds whenever  $\bar{b} = b^{-1}$ . That is, part (ii) holds whenever  $b$  lies on the unit circle between  $-i$  and  $i$ .

### Final remarks

(i) The speciality of the points  $x = \pm i$  for the function  $\psi_j(x)$  can be seen by writing

$$\begin{aligned}
\psi_j(x) &= (8\pi)^{-j} \sum_{n=1}^{\infty} H_{2j}(\sqrt{2\pi x n}) e^{-\pi n^2 x} = (8\pi)^{-j} \sum_{n=1}^{\infty} H_{2j}(\sqrt{2\pi x n}) e^{-\pi n^2 i} e^{-\pi n^2 (x-i)} \\
&= (8\pi)^{-j} \sum_{n=1}^{\infty} H_{2j}(\sqrt{2\pi x n}) (-1)^n e^{-\pi n^2 (x-i)} \\
&= -(8\pi)^{-j} \sum_{\substack{n=1 \\ n \text{ odd}}}^{\infty} H_{2j}(\sqrt{2\pi x n}) e^{-\pi n^2 (x-i)} + (8\pi)^{-j} \sum_{k=1}^{\infty} H_{2j}(\sqrt{2\pi x 2k}) e^{-4\pi k^2 (x-i)}. \quad (24)
\end{aligned}$$

(ii) The properties of a theta function have also been useful in an inverse scattering approach to the Riemann hypothesis (e.g. [9]). (iii) Proposition 4 offers a prospect for generalizing the very important Riemann-Siegel integral formula [12] that takes the form

$$\frac{2\xi(s)}{s(s-1)} = F(s) + \overline{F(1-\bar{s})}, \quad (25)$$

where  $F(s) = \pi^{-s/2} \Gamma(s/2) I(s)$  and  $I(s)$  is a certain contour integral taken over a straight line of slope  $-1$  crossing the real axis between 0 and 1 and directed from upper left to lower right.

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